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THEORETICAL RESEARCH UPON CHARGE TRANSFER
WITH INTERMEDIATE NITRIC OXIDE ION

H. Harvey Michels
United Technologies Research Center
East Hartford, Connecticut 06108

31 July 1979
Scientific Report No. 1

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entitled "Computations of Molecular Structures and
Transition Probabilities."

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Optimized ab initio calculations of the electronic structure of the $5\Sigma^+$ and 5Π states of the NO^+ molecular ion were carried out as part of our CY78 research effort. These calculations indicate that the lowest two $5\Sigma^+$ states have structure very similar to that found for the corresponding states of the isoelectronic N_2 molecule. The dominant configurations are $3\sigma_g^2 1\pi_u^2 1\pi_g^2$ [2220] and $3\sigma_g 1\pi_u^3 1\pi_g 3\sigma_u$ [1311], using homopolar labeling. These states strongly mix with the result that the upper $5\Sigma^+$ state, which connects to $\text{N}^+(^3\text{P}) + \text{O}(^3\text{P})$, becomes repulsive for internuclear separations shorter than $\sim 2.5\text{\AA}$. This state is therefore of secondary importance in the analysis of the charge transfer reaction $\text{N}^+(^3\text{P}) + \text{O}(^3\text{P}) \rightarrow \text{N}(^4\text{S}) + \text{O}^+(^4\text{S})$. The lowest 5Π state which crosses the lowest $5\Sigma^+$ state at $R=1.76\text{\AA}$ and which connects at long range to $\text{N}^+(^3\text{P}) + \text{O}(^3\text{P})$, is probably the most effective channel for charge transfer. Detailed calculations of the low-energy cross-section for charge transfer, based on this $5\Pi - 5\Sigma^+$ state coupling, are now complete. We find a cross-section of $1.7 \times 10^{-17} \text{ cm}^2$ @ 1.0 eV collision energy, in good agreement with Neynaber's experimental result ($1.3 \times 10^{-17} \text{ cm}^2$). The cross-section falls off exponentially for small values of collisional energy ($< 0.5\text{eV}$) where the reaction is apparently well described by the simple Landau-Zener solution.

A significant radiation component of $\text{N}^+ + \text{O}$ collision has been found. For 5 eV collision energies, we find a cross-section of $0.5 \times 10^{-19} \text{ cm}^2$ at $\lambda_{\text{max}} \sim 1220 \text{ nm}$. The reaction exhibits a broad wavelength dependence. Further studies including the possibility of radiative association of $\text{N}^+ + \text{O} \rightarrow \text{NO}^+ + h\nu$ are being investigated.

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ABSTRACT

Theoretical investigations of the electronic structure and radiative transition probabilities of atmospheric species and of kinetic reaction rates for electron-ion and atom-atom reactions are in progress. These studies are being performed using quantum mechanical methods and digital computer codes based on both ab initio methods, employing configuration-interaction (CI), and density functional methods, employing developments and extensions of models used previously in solid state calculations.

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Theoretical Research Investigation Upon
Reaction Rates to the Nitric Oxide
Positive Ion

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INTRODUCTION

The release of certain chemical species into the upper atmosphere results in luminous clouds that display the resonance electronic-vibrational-rotation spectrum of the released species. Such spectra are seen in rocket releases of chemicals for upper atmospheric studies and upon reentry into the atmosphere of artificial satellites and missiles. Of particular interest in this connection are the observed spectra of certain metallic oxides and air diatomic and triatomic species. From band intensity distribution of the spectra, and knowledge of the f-values for electronic and vibrational transitions, the local conditions of the atmosphere can be determined (Ref. 1).

Present theoretical efforts which are directed toward a more complete and realistic analysis of the transport equations governing atmospheric relaxation, including chemical effects, and the propagation of artificial disturbances require detailed information on atomic and ionic reaction rates and on thermal opacities and LWIR absorption in regions of temperature and pressure where molecular effects are important (Refs. 2 and 3). Although various experimental techniques have been employed for both atomic and molecular systems, theoretical studies have been largely confined to an analysis of the properties (bound-bound, bound-free and free-free) of atomic systems (Refs. 4 and 5). This has been due in large part to the unavailability of reliable wavefunctions for diatomic molecular systems, and particularly for excited states or states of open-shell structures. More recently, (Refs. 6-9) reliable theoretical procedures have been prescribed for such systems which have resulted in the development of practical computational programs.

The theoretical analysis of atmospheric reactions requires the knowledge of the electronic structure of atoms, ions and small molecular clusters of nitrogen and oxygen and the interaction of water or other small molecules with these clusters. Knowledge of the chemistry of metal oxide species, which might be present in a contaminated atmosphere, is also desired. In addition the basic collisional processes involving electrons, ions and neutral particles must be understood to evaluate the dynamic effects of the chemistry of the atmosphere. One important reaction is the charge transfer in $N^+ + O \rightarrow N + O^+$. This has been studied experimentally by Neynaber (Ref. 10 and 58) at collision energies between 0.5 eV and 25 eV but low energy (<0.5 eV) data are apparently extremely difficult to measure.

Because of the difficulty of conducting experiments to measure the appropriate cross sections for many thermal energy atmospheric processes, the development of a sound theoretical method for calculating low-energy cross sections appears necessary. Although relatively little work of this

nature has been done in the past, enough theoretical work is available to indicate that the development of such procedures can be made practical, particularly if good wave functions and potential energy curves are available for the interacting species.

The present research program was devoted to a theoretical study of the energetics and kinetic reaction rates of $N^+ + O$ collisions. The goal of this research program was to develop technical information concerning this system relevant to DNA interests in upper atmospheric reactions.

CURRENT STATUS OF QUANTUM MECHANICAL METHODS FOR DIATOMIC SYSTEMS

The application of quantum mechanical methods to the prediction of electronic structure has yielded much detailed information about atomic and molecular properties (Ref. 7). Particularly in the past few years, the availability of high-speed computers with large storage capacities has made it possible to examine both atomic and molecular systems using an ab initio approach, wherein no empirical parameters are employed (Ref. 11). Ab initio calculations for diatomic molecules employ a Hamiltonian based on the nonrelativistic electrostatic interaction of the nuclei and electrons, and a wavefunction formed by antisymmetrizing a suitable many-electron function of spatial and spin coordinates. For most applications it is also necessary that the wavefunction represent a particular spin eigenstate and that it have appropriate geometrical symmetry. Nearly all the calculations performed to date are based on the use of one-electron orbitals and are of two types: Hartree-Fock or configuration interaction (Ref. 8).

Hartree-Fock calculations are based on a single assignment of electrons to spatial orbitals, following which the spatial orbitals are optimized, usually subject to certain restrictions. Almost all Hartree-Fock calculations have been subject to the assumption that the diatomic spatial orbitals are all doubly occupied, as nearly as possible, and are all of definite geometrical symmetry. These restrictions define the conventional, or restricted, Hartree-Fock (RHF) method (Refs. 12 and 13). RHF calculations can be made with relatively large Slater-type orbital (STO) basis sets for diatomic molecules with first or second-row atoms, and the results are convergent in the sense that they are insensitive to basis enlargement. The RHF model is adequate to give a qualitatively correct description of the electron interaction in many systems, and in favorable cases can yield equilibrium interatomic separations and force constants. However, the double-occupancy restriction makes the RHF method inappropriate in a number of circumstances of practical interest. In particular, it cannot provide potential curves for molecules dissociating into odd-electron atoms (e.g., NO at large internuclear separation), or into atoms having less electron pairing than the original molecule [e.g., $O_2\ ^3\Sigma_g^- \rightarrow O(^3P)$]; it cannot handle excited states having unpaired electrons (e.g., the $^3\Sigma$ states of O_2 responsible for the Schumann-Runge bands); and, in general, it gives misleading results for molecules in which the extent of electron correlation changes with internuclear separation.

Configuration-interaction (CI) methods have the capability of avoiding the limitations of the RHF calculations. If configurations not restricted to doubly-occupied orbitals are included, a CI can, in principle, converge to an exact wave-function for the customary Hamiltonian. However, many CI

calculations have in fact been based on a restriction to doubly-occupied orbitals and therefore retain many of the disadvantages of the RHF method (Ref. 8). The use of general CI formulations involves three considerations, all of which have been satisfactorily investigated: the choice of basis orbitals, the choice of configurations (sets of orbital assignments), and the specific calculations needed to make wavefunctions describing pure spin states (Ref. 6). The first consideration is the art associated with quantum mechanical electronic structure calculations. Many methods (iterative NSO, perturbation selection, first order CI, etc.) have been advocated for the optimum choice of configurations. There are no firm rules at present and the optimum choice is a strong function of the insight of the particular research investigator. The last consideration, proper spin and symmetry projection, has proved difficult to implement, but computer programs have been developed for linear projection algebra at this Center, and the CI method has been found of demonstrable value in handling excited states and dissociation processes which cannot be treated with RHF techniques.

Either of the above described methods for ab initio calculations reduces in practice to a series of steps, the most important of which are the evaluation of molecular integrals, the construction of matrix elements of the Hamiltonian, and the optimization of molecular orbitals (RHF) or configuration coefficients (CI). For diatomic molecules, these steps are all comparable in their computing time, so that a point has been reached where there is no longer any one bottleneck determining computation speed. In short, the integral evaluation involves the use of ellipsoidal coordinates and the introduction of the Neumann expansion for the interelectronic repulsion potential (Ref. 14); the matrix element construction depends upon an analysis of the algebra of spin eigenfunctions (Ref. 15); and the orbital or configuration optimization can be carried out by eigenvalue techniques (Refs. 16, 17). All the steps have by now become relatively standard, and can be performed efficiently on a computer having 65,000 to 130,000 words of core storage, a cycle time in the microsecond range, and several hundred thousand words of peripheral storage.

Both the RHF and CI methods yield electronic wavefunctions and energies as a function of the internuclear separation, the RHF methods for one state, and the CI method for all states considered. The electronic energies can be regarded as potential curves, from which may be deduced equilibrium internuclear separations, dissociation energies, and constants describing vibrational and rotational motion (including anharmonic and rotation-vibration effects). It is also possible to solve the Schrödinger equation

for the motion of the nuclei subject to the potential curves, to obtain vibrational wavefunctions for use in transition probability calculations. The electronic wavefunctions themselves can be used to estimate dipole moments of individual electronic states, transition moments between different electronic states, and other properties. While all of the calculations described in this paragraph have been carried out on some systems, the unavailability of good electronic wavefunctions and potential curves has limited actual studies of most of these properties to a very small number of molecules.

METHOD OF APPROACH

Central to these studies are the actual quantum-mechanical calculations which must be carried out for the molecular species. For added clarity, various aspects of these calculations are discussed in individual subsections.

1. Levels of Approximation

Much evidence on diatomic and polyatomic systems indicates the near adequacy of a minimum Slater-type-orbital (STO) basis for constructing molecular wavefunctions (Refs. 18 and 19). This means inner-shell and valence-shell STO's of quantum numbers appropriate to the atoms (1s, 2s, 2p for C, N, O; 1s for H). The main deficiency of the minimum basis set is in its inability to describe polarization of π orbitals in atoms adjacent to H atoms, and successful calculations usually result if one (or a set) of p orbitals is supplied for each H atom. Values of the screening parameters ζ for each orbital can either be set from atomic studies or optimized in the molecule; the latter approach is indicated for studies of maximum precision. When high chemical accuracy is required, as for the detailed studies of the ground state of a system, a more extended basis should be used. Double-zeta plus polarization functions or optimized MO's usually are required.

The chosen basis sets give good results only when used in a maximally flexible manner. This implies the construction of CI wavefunctions with all kinds of possible orbital occupancies, so that the correlation of electrons into overall states can adjust to an optimum form at each geometrical conformation and for each state. Except when well-defined pairings exist for as many electrons as possible, a single-configuration study (even of Hartree-Fock quality) will be inadequate.

2. Spin and Symmetry

Proper electronic states for systems composed of light atoms should possess definite eigenvalues of the spin operator S^2 as well as an appropriate geometrical symmetry. The geometrical symmetry can be controlled by the assignment of orbitals to each configuration, but the spin state must be obtained by a constructive or projective technique. Formulas have been developed (Ref. 15) for projective construction of spin states from orthogonal orbitals, and programs implementing these formulas have for several years been in routine use at UTRC.

One of the least widely appreciated aspects of the spin-projection problem is that the same set of occupied spatial orbitals can sometimes be coupled to give more than one overall state of given S quantum number. It is necessary to include in calculations all such spin couplings, as the

optimum coupling will continuously change with changes in the molecular conformation. This is especially important in describing degenerate or near-degenerate excited electronic states.

3. Method of Ab Initio Calculation

A spin-free, nonrelativistic, electrostatic Hamiltonian is employed in the Born-Oppenheimer approximation. In systems containing atoms as heavy as N or O, this approximation is quite good for low-lying molecular states. For a diatomic molecule containing n electrons, the approximation leads to an electronic Hamiltonian depending parametrically on the internuclear separation. R :

$$\mathcal{H}(R) = -\frac{1}{2} \sum_{i=1}^n \nabla_i^2 - \sum_{i=1}^n \frac{Z_A}{r_{iA}} - \sum_{i=1}^n \frac{Z_B}{r_{iB}} + \frac{Z_A Z_B}{R} + \sum_{i>j}^n \frac{1}{r_{ij}} \quad (1)$$

where Z_A and Z_B are the charges of nuclei A and B, and r_{iA} is the separation of electron i and nucleus A. \mathcal{H} is in atomic units (energy in Hartrees, length in Bohrs).

Electronic wavefunctions $\psi(R)$ are made to be optimum approximations to solutions, for a given R , of the Schrödinger equation

$$\mathcal{H}(R)\psi(R) = E(R)\psi(R) \quad (2)$$

by invoking the variational principle

$$\delta W(R) = \delta \frac{\int \psi^*(R) \mathcal{H}(R) \psi(R) d\tau}{\int \psi^*(R) \psi(R) d\tau} \quad (3)$$

The integrations in Eq. (3) are over all electronic coordinates and the stationary values of $W(R)$ are approximations to the energies of states described by the corresponding $\psi(R)$. States of a particular symmetry are studied by restricting the electronic wavefunction to be a projection of the appropriate angular momentum and spin operators. Excited electronic states corresponding to a particular symmetry are handled by construction of configuration-interaction wavefunctions of appropriate size and form.

The specific form for $\psi(R)$ may be written

$$\psi(R) = \sum_{\mu} c_{\mu} \psi_{\mu}(R) \quad (4)$$

where each $\psi_{\mu}(R)$ is referred to as a configuration, and has the general structure

$$\psi_{\mu}(R) = A O_S \prod_{i=1}^n \psi_{\mu i}(r_i, R) \theta_M \quad (5)$$

where each $\psi_{\mu i}$ is a spatial orbital, A is the antisymmetrizing operator, O_S is the spin-projection operator for spin quantum number S , and θ_M is a product of α and β one-electron spin functions of magnetic quantum number M . No requirement is imposed as to the double occupancy of the spatial orbital, so Eqs. (4) and (5) can describe a completely general wavefunction.

In Hartree-Fock calculations $\psi(R)$ is restricted to a single ψ_u which is assumed to consist as nearly as possible of doubly-occupied orbitals. The orbitals $\psi_{\mu i}$ are then selected to be the linear combinations of basis orbitals best satisfying Eq. (3). Writing

$$\psi_{\mu i} = \sum_{\nu} a_{\nu i} \chi_{\nu} \quad (6)$$

The $a_{\nu i}$ are determined by solving the matrix Hartree-Fock equations

$$\sum_{\nu} F_{\lambda \nu} a_{\nu i} = \epsilon_i \sum_{\nu} S_{\lambda \nu} a_{\nu i} \quad (\text{each } \lambda) \quad (7)$$

where ϵ_i is the orbital energy of $\psi_{\mu i}$.

The Fock operator $F_{\lambda \nu}$ has been thoroughly discussed in the literature (Ref. 12) and depends upon one- and two-electron molecular integrals and upon the $a_{\nu i}$. This makes Eq. (7) nonlinear and it is therefore solved iteratively. UTRC has developed programs for solving Eq. (7) for both closed and open-shell systems, using basis sets consisting of Slater-type atomic orbitals. Examples of their use are in the literature (Ref. 6).

In configuration interaction calculations, the summation in Eq. (4) has more than one term, and the c_{μ} are determined by imposing Eq. (3), to obtain the secular equation

$$\sum_{\nu} (H_{\mu \nu} - w S_{\mu \nu}) c_{\nu} = 0 \quad (\text{each } \mu) \quad (8)$$

where

$$H_{\mu \nu} = \int \Psi_{\mu}^*(R) \mathcal{H}(R) \Psi_{\nu}(R) d\tau$$

$$S_{\mu \nu} = \int \Psi_{\mu}^*(R) \Psi_{\nu}(R) d\tau \quad (9)$$

Equation (7) is solved by matrix diagonalization using either a modified Givens method (Ref. 16) or a method due to Shavitt (Ref. 17).

The matrix elements $H_{\mu\nu}$ and $S_{\mu\nu}$ may be reduced by appropriate operator algebra to the forms

$$H_{\mu\nu} = \sum_P \epsilon_P \left\langle \theta_M \left| \mathcal{O}_S P \right| \theta_M \right\rangle \left\langle \prod_{i=1}^n \psi_{\mu i}(\underline{r}_i, R) \left| \mathcal{H}(R) P \right| \prod_{i=1}^n \psi_{\nu i}(\underline{r}_i, R) \right\rangle \quad (10)$$

$$S_{\mu\nu} = \sum_P \epsilon_P \left\langle \theta_M \left| \mathcal{O}_S P \right| \theta_M \right\rangle \left\langle \prod_{i=1}^n \psi_{\mu i}(\underline{r}_i, R) \left| P \right| \prod_{i=1}^n \psi_{\nu i}(\underline{r}_i, R) \right\rangle \quad (11)$$

where P is a permutation and ϵ_P its parity. The sum is over all permutations.

$\langle \theta_M | \mathcal{O}_S P | \theta_M \rangle$ is a "Sanibel coefficient" and the remaining factors are

spatial integrals which can be factored into one- and two-electron integrals. If the $\psi_{\mu i}$ are orthonormal, Eqs. (10) and (11) become more tractable and the $H_{\mu\nu}$ and $S_{\mu\nu}$ may be evaluated by explicit methods given in the literature (Ref. 15). Computer programs have been developed for carrying out this procedure, and they have been used for problems containing up to 40 total electrons, 10 unpaired electrons, and several thousand configurations.

The CI studies described above can be carried out for any orthonormal set of $\psi_{\mu i}$ for which the molecular integrals can be calculated. Programs developed by UTRC make specific provision for the choice of the $\psi_{\mu i}$ as Slater-type atomic orbitals, as symmetry molecular orbitals, as Hartree-Fock orbitals, or as more arbitrary combinations of atomic orbitals.

4. Molecular Integrals

The one- and two-electron integrals needed for the above described method of calculation are evaluated for STO's by methods developed by the present investigators (Ref. 20). All needed computer programs have been developed and fully tested at UTRC.

5. Configuration Selection

Using a minimum basis plus polarization set of one-electron functions, a typical system can have of the order of 10^4 configurations in full CI (that resulting from all possible orbital occupancies). It is therefore essential to identify and use the configurations describing the significant part of the wavefunction. There are several ways to accomplish this objective. First, one may screen atomic-orbital occupancies to eliminate those with excessive formal charge. Alternatively, in a molecular-orbital framework one may eliminate configurations with excessive numbers of anti-bonding orbitals. A third possibility is to carry out an initial screening

of configurations, rejecting those whose diagonal energies and interaction matrix elements do not satisfy significance criteria. Programs to sort configurations on all the above criteria are available at UTRC.

Other, potentially more elegant methods of configuration choice involve formal approaches based on natural-orbital (Ref. 21) or multiconfiguration SCF (Ref. 8) concepts. To implement the natural-orbital approach, an initial limited-CI wave-function is transformed to natural-orbital form, and the resulting natural orbitals are used to form a new CI. The hoped-for result is a concentration of the bulk of the CI wavefunction into a smaller number of significant terms. The multiconfiguration SCF approach is more cumbersome, but in principle more effective. It yields the optimum orbital choice for a pre-selected set of configurations. This approach works well when a small number of dominant configurations can be readily identified.

It should be emphasized that the problem of configuration choice is not trivial, and represents an area of detailed study in this research. The existence of this problem causes integral evaluation to be far from a unique limiting factor in the work.

6. Charge-Transfer Calculations

Even though low-energy atom-atom reactions play an important role in many physical processes, until recently comparatively little effort has been devoted to acquiring a knowledge of the appropriate cross sections. In the past, both theoreticians and experimental physicists have found it easier to study high-energy collisions. At these energies, the two colliding particles preserve their identities, and it is possible to treat the interaction between them as a perturbation. There is no guarantee that this procedure, known as the Born approximation, will always converge to the correct result (Ref. 22). As the energy of the colliding particles decreases, it is necessary to take account of the distortion these particles undergo during the collision. The method of perturbed stationary states was developed for calculating charge transfer and electronic excitation cross sections in relatively slow collisions between heavy particles (Ref. 23). The method has been presented in both wave and impact-parameter formalisms. In the first of these, the entire system is treated quantum-mechanically, while in the latter the nuclei are assumed to behave as classical particles, traveling along straight line trajectories, and the time-dependent Schrödinger equation is solved to calculate the probability of various types of electronic transitions (Refs. 24, 25, and 26). Forcing the particles to travel along straight lines limits the validity of the impact parameter method to collisions of several hundred electron-volts or greater (Ref. 27). The wave formulation of the method of perturbed stationary states appears to be one practical method of calculating thermal energy charge-exchange cross sections. A semi-classical close-coupling method (Ref. 28), based on an average scaling procedure, also offers utility for low to intermediate collision energies.

The use of the wave formalism to study charge-transfer reactions at thermal energies dates back to Massey and Smith's pioneering study of $\text{He}^+ + \text{He}$ thermal low-energy scattering (Ref. 29). Strictly speaking, their theory is applicable only to resonant charge transfer reactions, $A + A^+ \rightarrow A^+ + A$; however, it can be generalized to study nonresonant charge-transfer reactions as well as charge transfer into excited states. If the origin of coordinates is located at the center of mass of the nuclei of the colliding atoms, the Schrödinger equation for an atomic collision can be written in center-of mass coordinates as

$$(\mathbf{H} - E) \chi(\bar{\mathbf{r}}, \bar{\mathbf{R}}) = \left(\mathbf{H}_0 - \frac{\hbar^2}{2M} \nabla_{\bar{\mathbf{R}}}^2 - \frac{\hbar^2}{2M} \sum_i \sum_j \nabla_i \cdot \nabla_j - E \right) \chi(\bar{\mathbf{r}}, \bar{\mathbf{R}}) = 0 \quad (12)$$

where $\bar{\mathbf{r}}$ represents the position of the electrons, $\bar{\mathbf{R}}$ is the vector joining A to B, \mathbf{H}_0 is the Hamiltonian for the system when the nuclei are held fixed, M is the reduced mass of the two nuclei, \mathbf{M} is the sum of the nuclear masses, and E is the internal energy of the system, including the electronic energy.

Ignoring heavy particle kinetic energy terms in the center of mass system results in a modified form of the adiabatic approximation (Ref. 30) and yields perturbed molecular eigenfunctions $\psi_n(\vec{r}, \vec{R})$ which satisfy the equation

$$(H_0 - \frac{\hbar}{2M} \sum_i \sum_j \nabla_i \cdot \nabla_j) \psi_n(\vec{r}, \vec{R}) = \epsilon_n(R) \psi_n(\vec{r}, \vec{R}) \quad (13)$$

Here $\epsilon_n(R)$ is an electronic energy level of the molecule perturbed somewhat by the appearance of the cross terms. The wave function describing the colliding system, $X(\vec{r}, \vec{R})$ can be expanded as

$$X(\vec{r}, \vec{R}) = \sum_n \psi_n(\vec{r}, \vec{R}) F_n(\vec{R}) \quad (14)$$

The various scattering cross sections are determined by the asymptotic behavior of the $F_n(\vec{R})$. These functions are determined by substituting the expansion Eq. (14) into Eq. (12). Making use of the orthogonality of the molecular eigenfunctions, it is easy to derive the following set of coupled differential equations for the $F_n(R)$

$$\left(-\frac{\hbar^2}{2M} \nabla_{\vec{R}}^2 + V_n(\vec{R}) - \frac{\hbar^2 k_n^2}{2M} \right) F_n(\vec{R}) = \sum_m \frac{\hbar^2}{2M} \left\{ \langle \psi_n | \nabla_{\vec{R}}^2 | \psi_m \rangle F_m(\vec{R}) + 2 \langle \psi_n | \nabla_{\vec{R}} | \psi_m \rangle \cdot \nabla_{\vec{R}} F_m(\vec{R}) \right\} \quad (15)$$

where $V_n(R)$ and $\hbar^2 k_n^2 / 2M$ are the potential and kinetic energies of particles in the n^{th} channel. Many of the difficulties associated with trying to calculate thermal energy cross sections emanate from trying to derive and solve this infinite set of coupled partial differential equations. Until recently, the biggest obstacle in the calculation of low-energy cross sections has been the inability of theorists to develop accurate molecular eigenfunctions. For those problems for which the molecular eigenfunctions were available, the agreement between theory and experiment has been very reasonable for the amount of computational effort involved. This is true for spin exchange and excitation transfer reactions as well as resonance charge transfer reactions (Ref. 31-35).

Although the molecular wave functions and energies available in the past have not been sufficiently accurate to permit extension of the wave formalism to systems having more than about four electrons, recent advances in calculational techniques, especially for two-center systems, have largely overcome this problem. In particular, recent studies have demonstrated the possibility of producing highly accurate adiabatic electronic wave functions for systems containing as many as 40 electrons (Refs. 6, 36-38). The availability of these small but flexible wave functions, which have the property of connecting with the correct separated atomic states, increases

substantially the chances for successful and practical calculations of cross sections using the perturbed stationary state technique. This is especially true of charge transfer into excited states, where a knowledge of a number of the low-lying excited states is required.

Even with a reasonable number of the molecular eigenfunctions, the problem of calculating cross sections is far from solved; this is especially true of charge or excitation transfer into excited states. Many of the existing studies of symmetric resonance reactions are based on the two-state approximation which limits the number of terms in the expansion Eq. (14) to two. Under these conditions, the coupling terms on the right-hand side of Eq. (15) vanish (Ref. 39). We have, then, only to solve two partial differential equations, instead of a system of coupled equations. The situation is not as simple, however, for nonsymmetric reactions or for high-energy collisions involving excitation. For these problems, the coupling terms are the source of the transition and the coupled differential equations have to be solved directly.

While a great deal of effort has gone into deriving formal theories of inelastic and rearrangement collisions, relatively little work has gone into trying to solve the resulting equations. This is especially true of low-energy collisions, where the lack of good molecular wave functions has prevented people from evaluating the terms coupling the different channels. Previous studies which were part of the UTRC research program in the electronic structure of atoms and molecules have been devoted to calculating matrix elements similar to some of the terms coupling the electronic and nuclear motion. Some of the required work involves calculating derivatives of the electronic wave functions with respect to the internuclear distance. This task is made simpler by the use of compact but flexible wave functions such as those studied previously at this center.

The biggest obstacle to calculating low-energy cross sections is the solution of the infinite system or coupled partial differential equations describing the scattering, (Eq. 15). The physics of the problem usually serves as a guide to truncating these equations to a system of finite order. A partial wave expansion of the $F_n(\bar{R})$ leaves a large number of sets of coupled differential equations (Refs. 40 and 41). Since the number of equations increases as the collision energy increases, there is no single method for solving these equations. At thermal energies, a direct numerical integration of these equations is feasible (Refs. 42 and 43). At higher energies, when inelastic collisions and charge transfer into excited states becomes important, the trajectories of the incident and scattered particles may be nearly classical (Ref. 44). Under these conditions, it is often possible to use the W. K. B. wave function to obtain approximate solutions to these equations (Ref. 45).

7. Rotationally Induced Transition

Our studies of the electronic states of NO^+ which are important in the $\text{N}^+ + \text{O} \rightarrow \text{N} + \text{O}^+$ charge transfer reaction led primarily to consideration of the $^5\Sigma^+$ and $^5\Pi$ states of this molecular ion. The dominant reactant channel was found to be the lowest $^5\Pi$ state, which is bound, and the connecting charge transfer channel which has $^5\Sigma^+$ symmetry. For near-adiabatic collisions, this type of system can be handled using a semi-classical approach, directly solving the second order differential equations which couple the adiabatic levels, here of different angular momentum.

The adiabatic states $\psi_1(\underline{r}, R)$ and $\psi_2(\underline{r}, R)$ are eigenstates of the non-relativistic Hamiltonian, \mathcal{H} , for a fixed internuclear separation, R . We have

$$\mathcal{H} \phi_i(\underline{r}, R) = \epsilon_i \phi_i(\underline{r}, R) \quad i = 1, 2 \quad (16)$$

In the two-state approximation we have, using impact parameter formulation,

$$\begin{aligned} \psi = & c_1(t) \phi_1(\underline{r}, R) e^{-i/\hbar \int_0^t \epsilon_1 d\tau} \\ & + c_2(t) \phi_2(\underline{r}, R) e^{-i/\hbar \int_0^t \epsilon_2 d\tau} \end{aligned} \quad (17)$$

where $R = R(t)$ and is defined by the collision trajectory.

We now require the inner product of ψ and ϕ_i to vanish over the electronic coordinates

$$\langle \phi_1 | \mathcal{H} - i\hbar \frac{\partial}{\partial t} | \psi \rangle = 0 \quad (18a)$$

$$\langle \phi_2 | \mathcal{H} - i\hbar \frac{\partial}{\partial t} | \psi \rangle = 0 \quad (18b)$$

Combining Eqs. (16), (17), and (18), we have

$$\begin{aligned} \left[\frac{\partial c_1}{\partial t} + c_1 \langle \phi_1 | \frac{\partial \phi_1}{\partial t} \rangle \right] e^{-i/\hbar \int_0^t \epsilon_1 d\tau} \\ + c_2 \langle \phi_1 | \frac{\partial \phi_2}{\partial t} \rangle e^{-i/\hbar \int_0^t \epsilon_2 d\tau} = 0 \end{aligned} \quad (19a)$$

$$\begin{aligned} \left[\frac{\partial c_2}{\partial t} + c_2 \langle \phi_2 | \frac{\partial \phi_2}{\partial t} \rangle \right] e^{-i/\hbar \int_0^t \epsilon_2 d\tau} \\ + c_1 \langle \phi_2 | \frac{\partial \phi_1}{\partial t} \rangle e^{-i/\hbar \int_0^t \epsilon_1 d\tau} = 0 \end{aligned} \quad (19b)$$

Converting from differentiation with respect to time, to velocity and angular momentum, we have

$$\frac{\partial \phi_i}{\partial t} = \frac{\partial R}{\partial t} \frac{\partial \phi_i}{\partial R} + \frac{i}{\hbar} \frac{\partial V_\theta}{\partial t} L_T \phi_i \quad (20)$$

where V_θ is the angular velocity of the internuclear axis and L_T is the angular momentum coupling operator. The first term on the RHS of Eq. (20) leads to the well known Landau-Zener (Ref. 46) solution for states of identical molecular symmetry. For such cases the second term in Eq. (20) vanishes.

For the system under study here, only the second term on the RHS of Eq. (20) contributes in Eqs. (19) and we are led to the following coupled equations,

$$\frac{\partial c_1}{\partial t} + \frac{i}{\hbar} \frac{\partial V_\theta}{\partial t} c_2 \langle \phi_1 | L_T | \phi_2 \rangle e^{-\frac{i}{\hbar} \int_0^t (\epsilon_2 - \epsilon_1) d\tau} = 0 \quad (21a)$$

$$\frac{\partial c_2}{\partial t} + \frac{i}{\hbar} \frac{\partial V_\theta}{\partial t} c_1 \langle \phi_2 | L_T | \phi_1 \rangle e^{-\frac{i}{\hbar} \int_0^t (\epsilon_1 - \epsilon_2) d\tau} = 0 \quad (21b)$$

Assuming a linear dependence of ϵ on R near the crossing point of the collision, we have

$$\epsilon_2 - \epsilon_1 = b\hbar(R - R_x) = \alpha t \quad (22)$$

$$\alpha = \frac{V_R}{\hbar} \left. \frac{d(\epsilon_2 - \epsilon_1)}{dR} \right|_{R_x} \quad (23)$$

Assuming also that $\langle \phi_1 | L_T | \phi_2 \rangle = \langle L_T \rangle$ is essentially constant over the dominant region of the collision, we have

$$\frac{\partial c_1}{\partial t} + \frac{iW \langle L_T \rangle}{\hbar} c_2 e^{-\frac{i}{\hbar} \int_0^t (\epsilon_2 - \epsilon_1) d\tau} = 0 \quad (24a)$$

$$\frac{\partial c_2}{\partial t} + \frac{iW \langle L_T \rangle}{\hbar} c_1 e^{-\frac{i}{\hbar} \int_0^t (\epsilon_1 - \epsilon_2) d\tau} = 0 \quad (24b)$$

Equations (24a) and (24b) have been solved numerically by Russek (Ref. 47) for the case of curve-crossing states with $\Delta\Lambda = \pm 1$. For small values of angular velocity, Russek shows that Eq. (24) reduces to a standard Landau-Zener form. For large velocities, the general solution of Eq. (24) must be employed.

DISCUSSION OF RESULTS

The absorption coefficient for the NO^+ fundamental vibration-rotation band has recently been measured by Bien, et al. (Ref. 48). The reported integrated value is $140 \text{ cm}^{-2} \text{ atm}^{-1}$ in conflict with previous experimental estimates of $500 \text{ cm}^{-2} \text{ atm}^{-1}$ (Ref. 49) and a recent theoretical value of $89 \text{ cm}^{-2} \text{ atm}^{-1}$ (Ref. 50). Since the dominant atmospheric molecular ion above 100 km is NO^+ , its radiation characteristics and interactions with electrons and other atomic and molecular species are of primary importance in understanding the detailed chemistry of the atmosphere. Relatively little is known about the excited electronic states of the NO^+ ion. Accurate potential curves are available for the ground $X^1\Sigma^+$ state and for the $A^1\Pi$ and $a^3\Sigma^+$ excited states of NO^+ (Ref. 51). Gilmore also gives some experimental estimates of other excited states of NO^+ . More recently Thulstrup, et al. (Refs. 52 and 53) have assigned additional excited states of NO^+ based on photoelectron spectrum. A summary of these data is shown in Fig. 1. A correlation diagram for some of the low-lying valence excited states of NO^+ is shown in Table 1. In addition to these valence excited states there exists a large manifold of Rydberg states to the $\text{N}^+(^3P) + \text{O}^+(^4S)$ limit. The energies of the dissociation limits of the low-lying electronic states of NO^+ are shown in Table 2. It is obvious that only a small fraction of the low-lying excited states for this system have been experimentally investigated.

Few theoretical studies have been carried out for the excited states of this system. Lefebvre-Brion and Moser (Refs. 54 and 55) have studied the lowest-lying $^1\Pi$ and $^3\Pi$ states in an SCF framework. More recently, Thulstrup and Öhrn (Refs. 52 and 53) have examined low-lying singlet and triplet states of Σ^+ , Σ^- , Π and Δ symmetry. Their studies excluded higher spin and angular momentum states which may be important in perturbation analysis. Also, their calculations for $^3\Pi$, $^1\Sigma$ and $^3\Sigma$ symmetries were truncated in expansion length owing to their computer program limitations. Their predicted locations for these states are not in good agreement with the best experimental estimates.

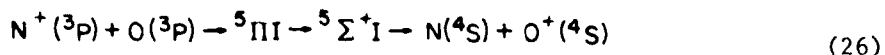
A complete and quantitatively uniform *ab initio* CI study of all the low-lying valence states of NO^+ was conducted under this program. This study was similar to that carried out for the 102 low-lying valence states of the nitrogen molecule (Ref. 56). Many of the states are similar since NO^+ is isoelectronic with N_2 .

These calculations have the property of correct dissociation to atomic limits and, as previously found for the N_2 system, a gradual and uniformly increasing correlation error with decreasing internuclear separation. This error arises from inadequacy of the basis set to fully describe polarization effects between the core and valence electrons. This error is quantitatively similar for the excited low-lying states of a given symmetry and our calculated potential curves have therefore been empirically adjusted to yield agreement with RKR curves constructed from the limited known spectroscopic data. This empirical adjustment takes the simple form;

$$\Delta E(R) = E(R)_{\text{calc.}} - E(R)_{\text{exp.}} \quad (25)$$

We find that ΔE is a strongly increasing function of R and dominant molecular orbital configuration for short internuclear separations but is nearly independent of the spin state. Thus, nearly universal correction curves (error $\sim .2$ eV) exist for most of the NO^+ valence excited states.

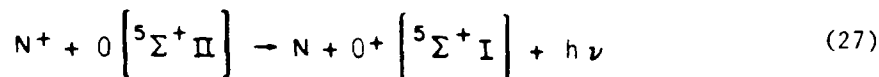
Empirically adjusted potential energy curves for NO^+ based on previous ab initio calculations and the available experimental spectroscopic data have been derived for studies of the radiation characteristics of the strongest electronic transitions of NO^+ (Ref. 57). Additional, more refined studies of the symmetries of NO^+ connecting to $N^+(^3P) + O(^3P)$ and $N(^4S) + O(^4S)$ were required for the present charge transfer problem. These calculations are shown in Fig. 1 along with the known spectroscopic states of NO^+ . We find that coupling of the $^5\Pi$ and $^5\Sigma^+$ states are probably the most effective channels for the charge transfer reaction



Optimized ab initio calculations of the electronic structure of the $^5\Sigma^+$ and $^5\Pi$ states of the NO^+ molecular ion were then carried out. These calculations indicate that the lowest two $^5\Sigma^+$ states have structure very similar to that found for the corresponding states of the isoelectronic N_2 molecule. The dominant configurations are $3\sigma_g^2 1\pi_u^2 1\pi_g^2$ (2220) and $3\sigma_g^2 1\pi_u^3 1\pi_g 3\sigma_u$ (1311), using homopolar labeling. These states strongly mix with the result that the upper $^5\Sigma^+$ state, which connects to $N^+(^3P) + O(^3P)$, becomes repulsive for internuclear separations shorter than $\sim 2.5 \text{ \AA}$. This state is therefore of secondary importance in the analysis of the charge transfer reaction $N^+(^3P) + O(^3P) \rightarrow N(^4S) + O(^4S)$. The lowest $^5\Pi$ state, which crosses the lowest $^5\Sigma^+$ state at $R=1.75 \text{ \AA}$ and which connects at long range to $N^+(^3P) + O(^3P)$, is therefore the only effective channel for charge transfer. A detailed picture of the NO^+ states of quintet symmetry is shown in Fig. 2.

Through the use of these calculated potential curves and corresponding eigenfunctions we have been able to evaluate the cross-section for charge transfer in $N^+ + O$ collisions with the method outlined in Section 7 above. In Fig. 3, we show the reduced cross-section as a function of reduced velocity, $y = hv/bR_x^2$, for Reaction (26). Also shown are Neynaber's recent experimental data (Ref. 58) and a value deduced by Dalgarno (Ref. 59) from Atmosphere Explorer data (Refs. 60 and 61). We find a cross-section of $1.7 \times 10^{-17} \text{ cm}^2$ @ 1.0 eV collision energy, in good agreement with Neynaber's experimental result ($1.3 \times 10^{-17} \text{ cm}^2$). The cross-section falls off exponentially for small values of the collisional energy ($< 0.5 \text{ eV}$), where the reaction is apparently well described by the simple Landau-Zener solution.

In addition to the direct collisional cross-section, we have investigated the possible radiative component corresponding to



For 5 eV collision energy, we find a cross-section of $0.5 \times 10^{-19} \text{ cm}^2$ at $\lambda_{\text{max}} \sim 1220 \text{ nm}$, using a modified Franck-Condon code for radiative transitions between unbound states. The reaction exhibits a broad wavelength dependence owing to the mixing of eigenfunctions for ${}^5\Sigma^+I$ and ${}^5\Sigma^+\Pi$ over a large range of internuclear separation.

Further studies including the possibility of radiative association of $N^+ + O \rightarrow NO^+ + h\nu$ are presently under investigation.

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TABLE 1
LOW-LYING MOLECULAR STATES OF NO⁺ AND THEIR
DISSOCIATION LIMITS

<u>Dissociation Limit</u>	<u>Molecular States</u>
N(⁴ S _u) + O ⁺ (⁴ S _u)	1 _Σ ⁺ (1), 3 _Σ ⁺ (1), 5 _Σ ⁺ (1), 7 _Σ ⁺ (1)
N ⁺ (³ P _g) + O(³ P _g)	1 _Σ ⁺ (2), 3 _Σ ⁺ (2), 5 _Σ ⁺ (2), 1 _Σ ⁻ (1), 3 _Σ ⁻ (1), 5 _Σ ⁻ (1), 1 _Π (2), 3 _Π (2), 5 _Π (2), 1 _Δ (1), 3 _Δ (1), 5 _Δ (1)
N(² D _u) + O ⁺ (⁴ S _u)	3 _Σ ⁺ (1), 5 _Σ ⁺ (1), 3 _Π ⁺ (1), 5 _Π (1), 3 _Δ (1), 5 _Δ (1)
N(⁴ S _u) + O ⁺ (² D _u)	3 _Σ ⁺ (1), 5 _Σ ⁺ (1), 3 _Π (1), 5 _Π (1), 3 _Δ (1), 5 _Δ (1)
N(² P _u) + O ⁺ (⁴ S _u)	3 _Σ ⁻ (1), 5 _Σ ⁻ (1), 3 _Π (1), 5 _Π (1)
N ⁺ (¹ D _g) + O(³ P _g)	3 _Σ ⁺ (1), 3 _Σ ⁻ (2), 3 _Π (3), 3 _Δ (2), 3 _Φ (1)
N(⁴ S _u) + O ⁺ (² P _u)	3 _Σ ⁻ (1), 5 _Σ ⁻ (1), 3 _Π (1), 5 _Π (1)
N ⁺ (³ P _g) + O(¹ D _g)	3 _Σ ⁺ (1), 3 _Σ ⁻ (2), 3 _Π (3), 3 _Δ (2), 3 _Φ (1)
N ⁺ (¹ S _g) + O(³ P _g)	3 _Σ ⁻ (1), 3 _Π (1)

TABLE 1 (Cont'd)
LOW-LYING MOLECULAR STATES OF NO^+ AND THEIR
DISSOCIATION LIMITS

<u>Dissociation Limit</u>	<u>Molecular States</u>
$\text{N}(^2\text{D}_u) + \text{O}^+(^2\text{D}_u)$	$^1\Sigma^+(3), ^3\Sigma^+(3), ^1\Sigma^-(2),$ $^3\Sigma^-(2), ^1\Pi(4), ^3\Pi(4),$ $^1\Delta(3), ^3\Delta(3), ^1\Phi(2),$ $^3\Phi(2), ^1\Gamma(1), ^3\Gamma(1)$
$\text{N}^+(^1\text{D}_g) + \text{O}(^1\text{D}_g)$	$^1\Sigma^+(3), ^1\Sigma^-(2), ^1\Pi(4),$ $^1\Delta(3), ^1\Phi(2), ^1\Gamma(1)$
$\text{N}^+(^3\text{P}_g) + \text{O}(^1\text{S}_g)$	$^3\Sigma^-(1), ^3\Pi(1)$

TABLE 2

ENERGIES OF NITROGEN AND OXYGEN ATOMIC AND IONIC STATES REPRESENTING
DISSOCIATION LIMITS OF LOW-LYING NO^+ STATES

Atomic and Ionic States (Experimental order)	Total Energy (Hartrees)	Energy Relative to $^4\text{S}_\text{u} + ^4\text{S}_\text{u}$ (eV)	
		Calc.	Exp.
$\text{N}(^4\text{S}_\text{u}) + \text{O}^+(^4\text{S}_\text{u})$	-128.42277	0.000	0.000
$\text{N}^+(^3\text{P}_\text{g}) + \text{O}(^3\text{P}_\text{g})$	-128.31777	2.857	0.916
$\text{N}(^2\text{D}_\text{u}) + \text{O}^+(^4\text{S}_\text{u})$	-128.30317	3.255	2.383
$\text{N}^+(^1\text{D}_\text{g}) + \text{O}(^3\text{P}_\text{g})$	-128.23804	5.027	2.815
$\text{N}^+(^3\text{P}_\text{g}) + \text{O}(^1\text{D}_\text{g})$	-128.22386	5.413	2.883
$\text{N}(^4\text{S}_\text{u}) + \text{O}^+(^2\text{D}_\text{u})$	-128.28190	3.833	3.325
$\text{N}(^2\text{P}_\text{u}) + \text{O}^+(^4\text{S}_\text{u})$	-128.26192	4.377	3.575
$\text{N}^+(^1\text{D}_\text{g}) + \text{O}(^1\text{D}_\text{g})$	-128.14412	7.583	4.782
$\text{N}^+(^1\text{S}_\text{g}) + \text{O}(^3\text{P}_\text{g})$	-128.17437	6.759	4.968
$\text{N}(^4\text{S}_\text{u}) + \text{O}^+(^2\text{P}_\text{u})$	-128.22932	5.264	5.016
$\text{N}^+(^3\text{P}_\text{g}) + \text{O}(^1\text{S}_\text{g})$	-128.14286	7.617	5.105
$\text{N}(^2\text{D}_\text{u}) + \text{O}^+(^2\text{D}_\text{u})$	-128.16229	7.088	5.708

FIG. 1

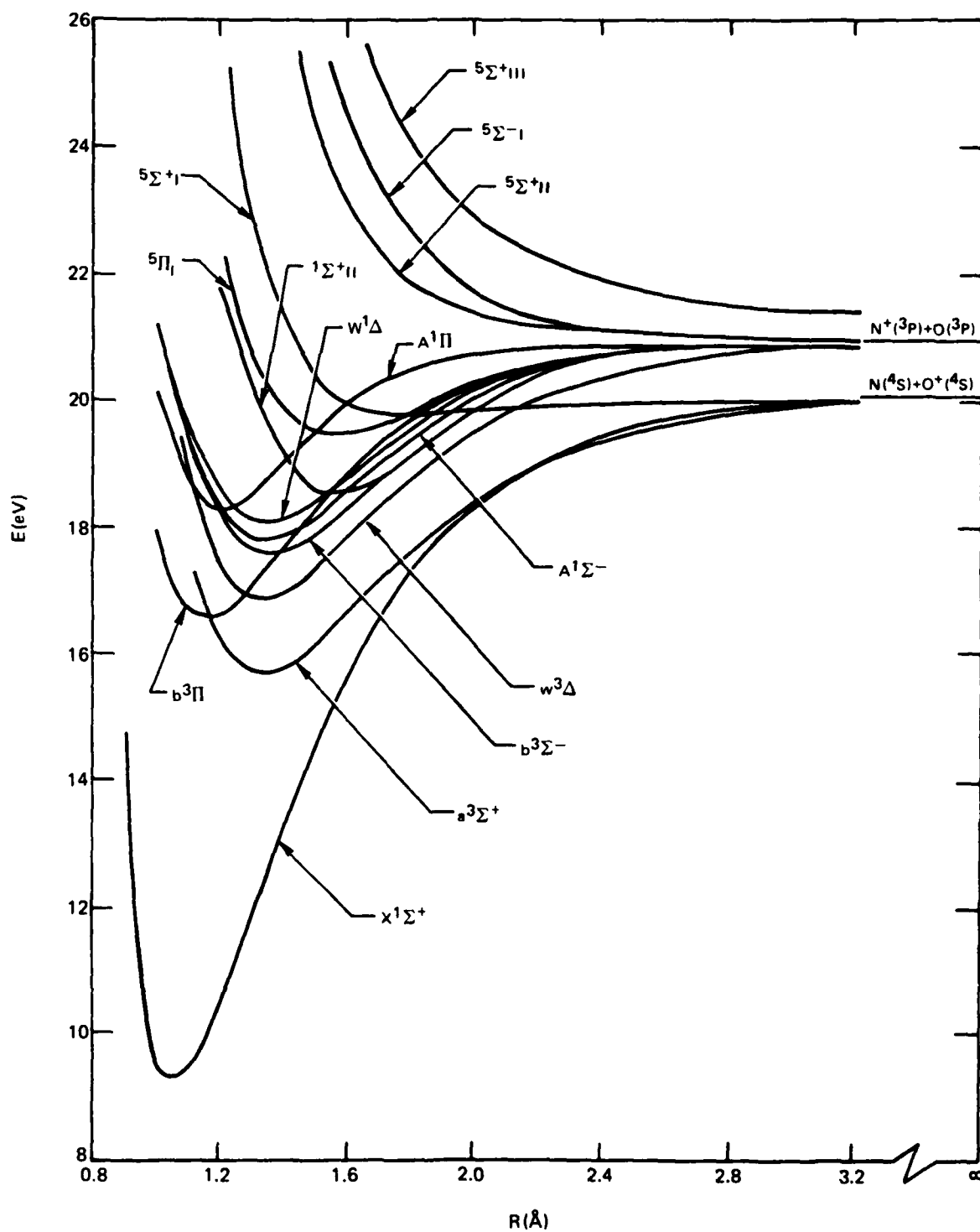
LOW-LYING POTENTIAL ENERGY CURVES OF NO^+ 

FIG. 2

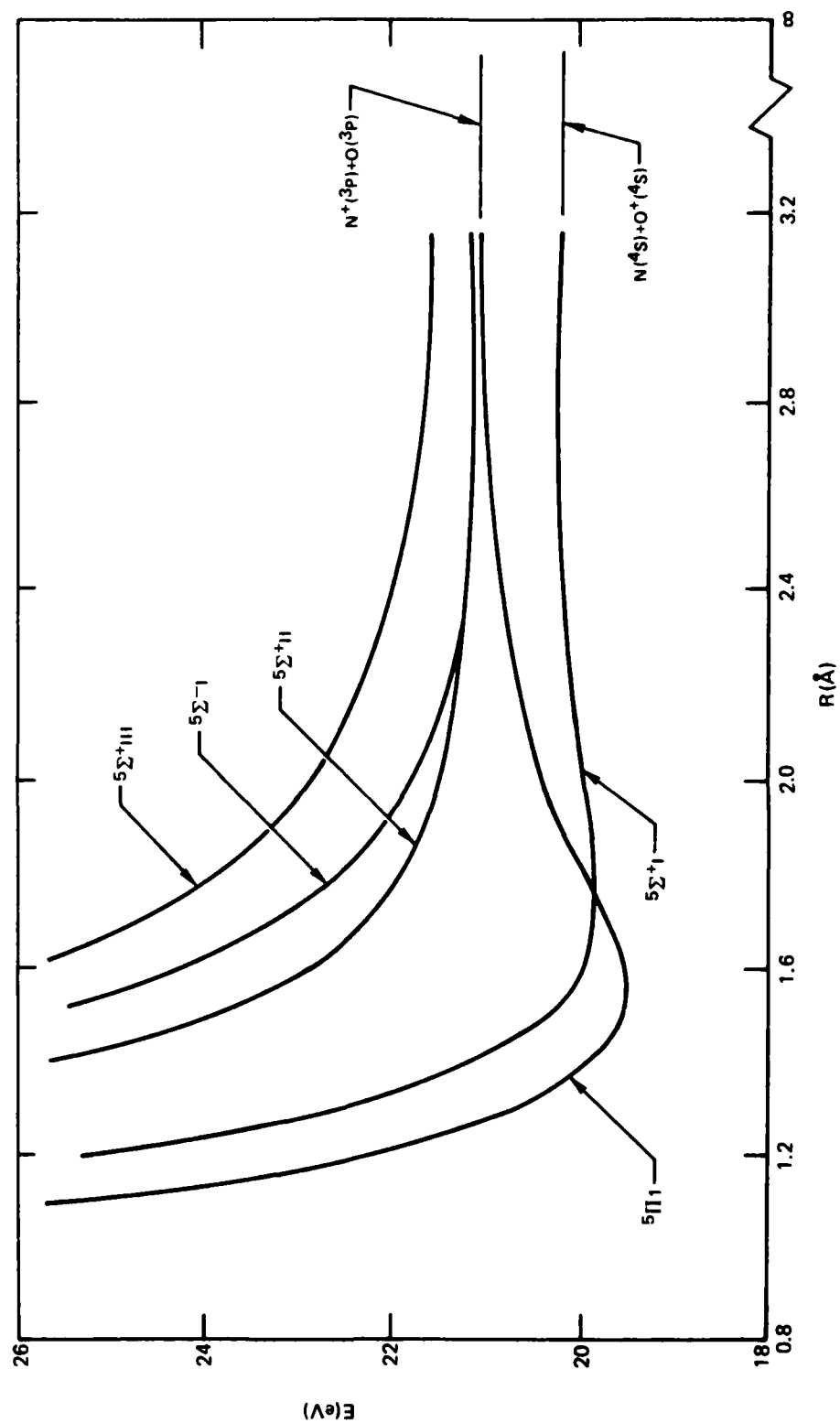
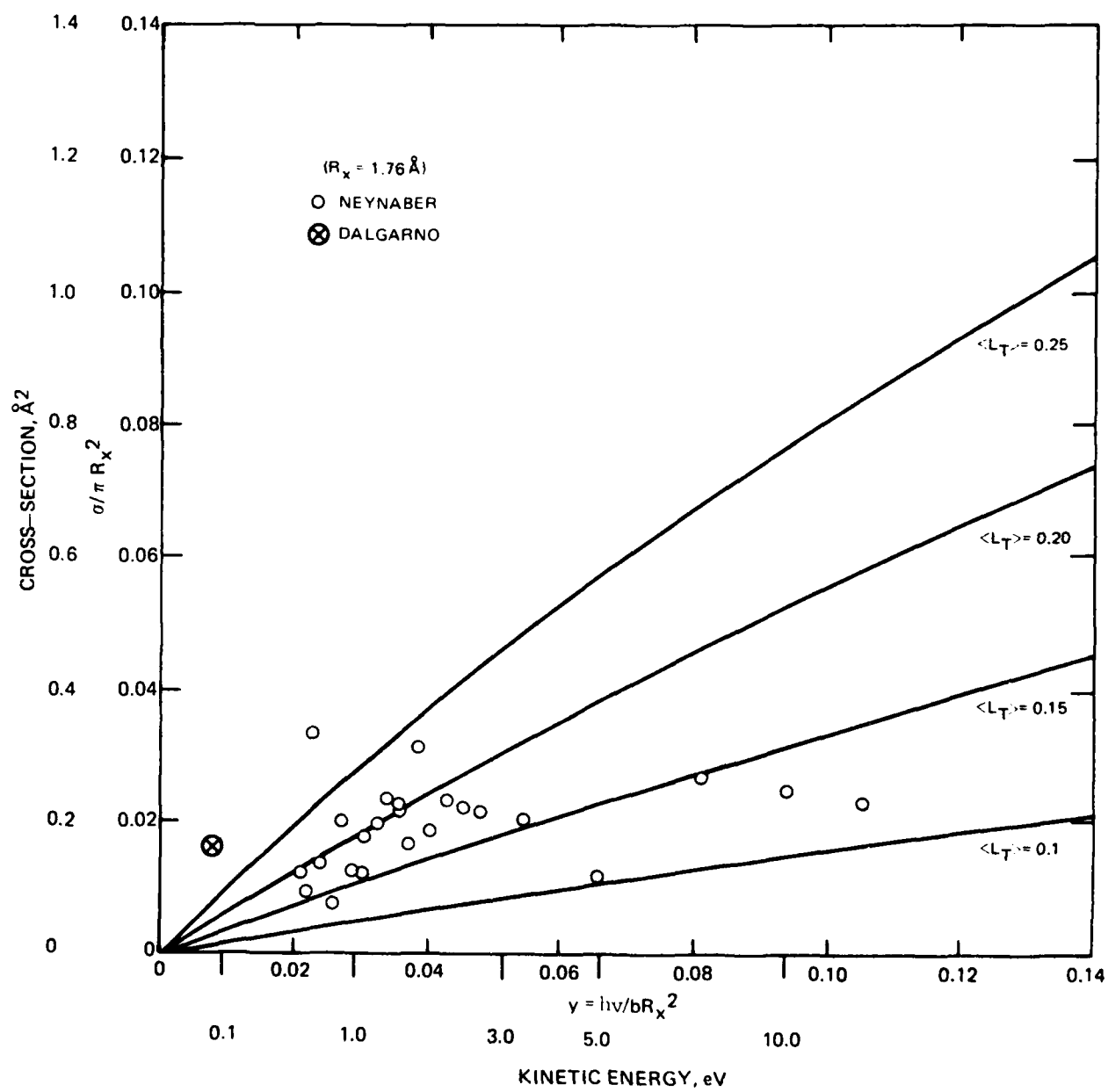
LOW-LYING $5\Sigma^+$ AND 5Π STATES OF NO^+ 

FIG. 3

COLLISION CROSS-SECTION FOR ROTATIONAL EXCITATION



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